Paraldehyde

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 8.50e-01

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found
Paraldehyde
Measured: 0.67
Predicted: 8.50e-01

Image not found
Ethyl orthoformate
Measured: 1.20
Predicted: 1.05

Image not found
Methyl pivalate
Measured: 1.83
Predicted: 1.76

Image not found
Metaldehyde acetaldehyde tetramer
Measured: 0.12
Predicted: 4.47e-01

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Butanoic acid, 3-methyl-, methyl ester
Measured: 1.82
Predicted: 1.83